

PATENT

58. The computer implemented system of claim 57, wherein the spectral data is calculated  $^{13}\text{C}$  NMR data.

59. The method of claim 27, wherein the endpoint data is selected from the group consisting of quantitative endpoint data, qualitative endpoint data, and combinations thereof.

60. The method of claim 30, wherein the spectral data is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.

61. The method of claim 41, wherein the spectral data is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.

62. The method of claim 48, wherein the endpoint data is selected from the group consisting of quantitative endpoint data, qualitative endpoint data, and combinations thereof.

63. The method of claim 49, wherein the spectral data is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.

64. The method of claim 52, wherein the spectral data is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.--

**Remarks:**

Support for new claims 55-58, 60-61, and 63-64 is found on page 21, lines 10-20. Additional support is found in Example 5 (page 55, line 17 to page 56, line 28). Further support for these new claims is found on page 63, lines 3-14.